Chapter

3

Single Variable Unconstrained Optimization Methods

3.1 Introduction

A function $f(x)$ is described as the relation between the input and output variables of a system. In a very basic sense, it is a correlation that provides a unique value of $y = f(x)$ for every choice of x. In this situation, x is termed as the independent variable whereas, y is called the dependent variable. The dependent variables vary with the change of independent variables. The thermal conductivity of any material changes with temperature; here, temperature is independent variable whereas thermal conductivity is the dependent variable. Mathematically, we can represent a set $S \subset R$, where R Rrepresents the set of all real numbers. A correspondence or a transformation can be defined by certain correlation that gives a single numerical value to all points $S \in R$. This type of relationship is called a scalar function f defined on the set S.

When, the set $S = R$, we have an unconstrained function of one variable. On the other hand, we can define a function on a constrained region whenever S is a proper subset of R. For example,

$$f(x) = 2x^3 + 5x^2 - 3x + 2 \text{ for all } x \in R \tag{3.1}$$

is an unconstrained function, while

$$f(x) = 2x^3 + 5x^2 - 3x + 2 \text{ for all } x \in S = \{x | -5 \leq x \leq 5\} \tag{3.2}$$

is a constrained function.

In this chapter, we will discuss different methods for single variable unconstrained problem.

3.2 Optimization of Single Variable Function

An appropriate method for the optimization of a function with single variable is necessary for two main reasons:

i. A number of unconstrained problems intrinsically involve only one variable (Example: 3.3)

ii. One-dimensional search is repeatedly used during the optimization of unconstrained and constrained optimization problems (e.g., univariate method).

3.2.1 Criteria for optimization

A single variable function $f(x)$ is supposed to have a local or relative minimum at $x = x^*$ if $f(x^*) \leq f(x^* + h)$ for all positive and negative values of h which is sufficiently small. Correspondingly, a point x^* is said t have a local or relative maximum when $f(x^*) \geq f(x^* + h)$ for all values of h is very close to zero. A function $f(x)$ is called a absolute or global minimum at the point x^* when $f(x^*) \leq f(x)$ for all x; not only for all x close to x^* but, also in the domain over which $f(x)$ is defined. Likewise, if $f(x^*) \geq f(x)$ for all values of x in the domain then the point x^* will be a global maximum of $f(x)$. Figure 3.1 shows various local and global optimum points.

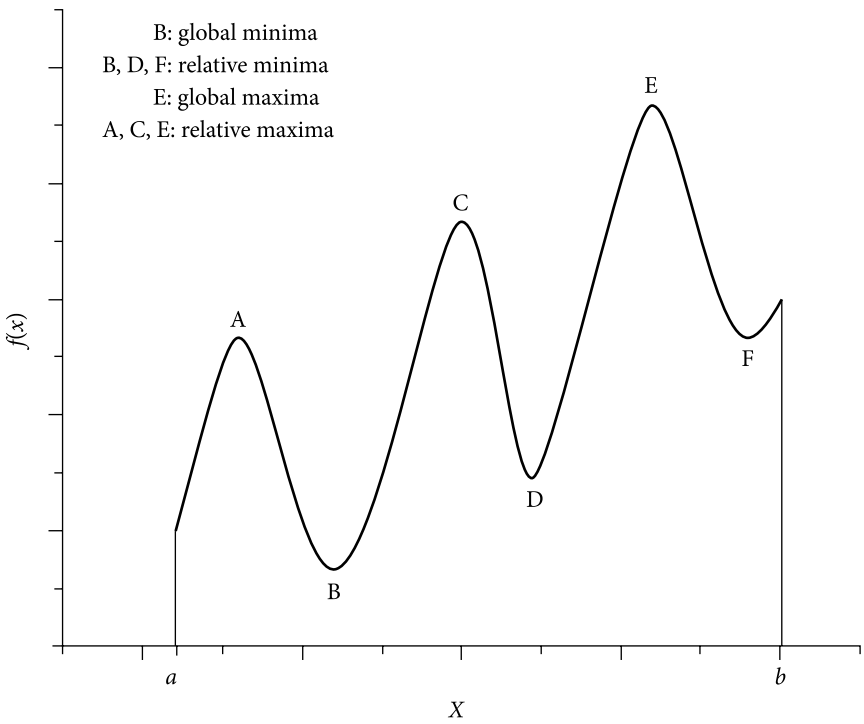

Fig. 3.1 Global and relative optimum points

For an optimization problem with single-variable, we need to find the value of $x = x^*$ in the interval $[a, b]$ such that x^* minimizes the function $f(x)$. This interval $[a, b]$ is considered for initial calculation of the static point. The global optimum point may be outside this interval. For a single

variable function, the necessary and sufficient conditions for the relative minimum are given in the following two theorems.

Theorem 3.1

Necessary Condition

If a function $f(x)$ is defined in the interval $a \le x \le b$ and possesses a relative minimum at the point $x = x^*$, where $a \le x^* \le b$, and if the derivative $df(x)/dx = f'(x)$ exists as a finite number at $x = x^*$, then $f'(x) = 0$.

Proof

By the definition we know that

$$f'\left(x^*\right) = \lim_{h \to 0} \frac{f\left(x^* + h\right) - f\left(x^*\right)}{h} \tag{3.3}$$

exists as a definite number, which we require to shown to be zero. As the point x^* is a relative minimum, we can write

$$f\left(x^*\right) \le f\left(x^* + h\right) \tag{3.4}$$

When, the all values of h are sufficiently close to zero, we have

$$\frac{f\left(x^* + h\right) - f\left(x^*\right)}{h} \ge 0 \quad \text{if } h > 0 \tag{3.5}$$

$$\frac{f\left(x^* + h\right) - f\left(x^*\right)}{h} \le 0 \quad \text{if } h < 0 \tag{3.6}$$

Thus, Eq. (3.3) provides the limit as h tends to zero through positive values as

$$f'\left(x^*\right) \ge 0 \tag{3.7}$$

at the same time as it provides the limit as h approaches to zero through negative values as

$$f'\left(x^*\right) \le 0 \tag{3.8}$$

both the Eqs (3.7) and (3.8) will be satisfied only when

$$f'\left(x^*\right) = 0 \tag{3.9}$$

Therefore, the theorem is proved.

Limitations

i. This theorem does not give any idea what happens when a maximum or minimum occurs at a point x^* where the derivative does not exist. For example, it is clear in Fig. 3.2 that the value of the derivative varies depending on whether h moves toward zero through negative or positive values, respectively.

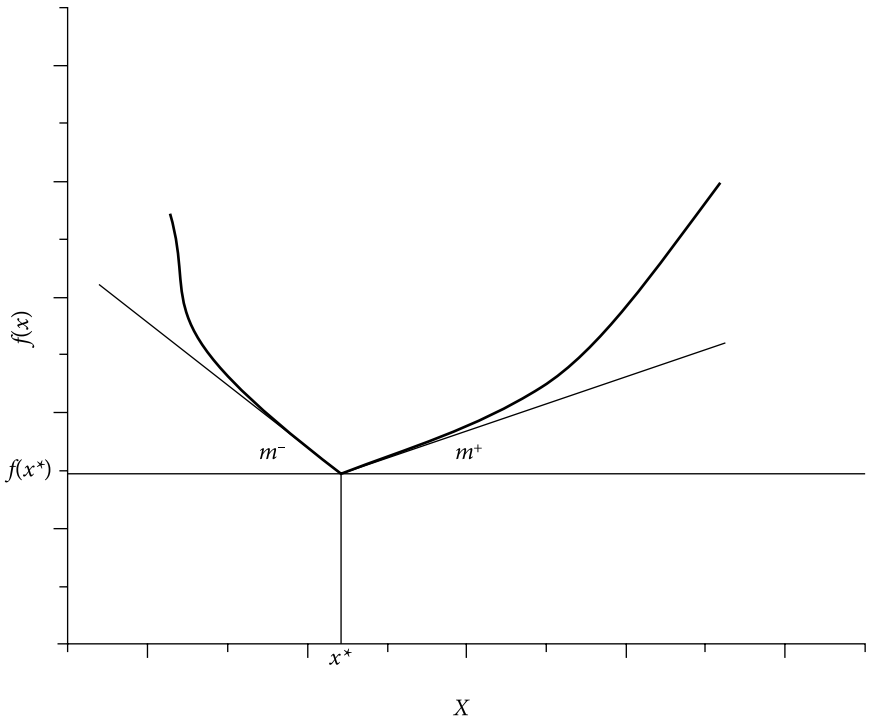

Fig. 3.2 Undefined derivative at x^*

The derivative $f'(x^*)$ fail to exist unless the numbers m^- and m^+ are equal. If $f'(x^*)$ does not exist, the Theorem 3.1 is not applicable.

A function $f(x)$, well defined at $x = x^*$. The point $x = x^*$ is called *critical point* if the derivative of $f(x)$ does not exist at that point. Consider, the function $f(x) = x^{2/3}$; derivative of this function is $f'(x) = \frac{2}{3}x^{-1/3}$. The derivative of $f(x)$ does not exist when $x = 0$ since, the denominator then takes the value 0. The point, $x = 0$ is therefore, a critical point of $f(x)$.

ii. A maximum or minimum can arises at an endpoint of the interval within which the function is defined; however, this theorem does not state what happens for this situation. In this case, the term

$$\lim_{h \to 0} \frac{f(x^* + h) - f(x^*)}{h} \tag{3.10}$$

exists only for negative values of h or for positive values of h, and for this reason the derivative is not defined at the endpoints.

iii. By this theorem, it is not inevitable that the function will have a maximum or minimum at every point wherever the derivative is zero. For instance, as shown in Fig. 3.3, the derivative of the function $f'(x^*) = 0$ at $x = 0$. However, this point is neither a maximum nor a minimum. Generally, a point x^* at which $f'(x^*) = 0$ is known as *stationary point*. A stationary point may be a maximum, minimum, or an inflection point.

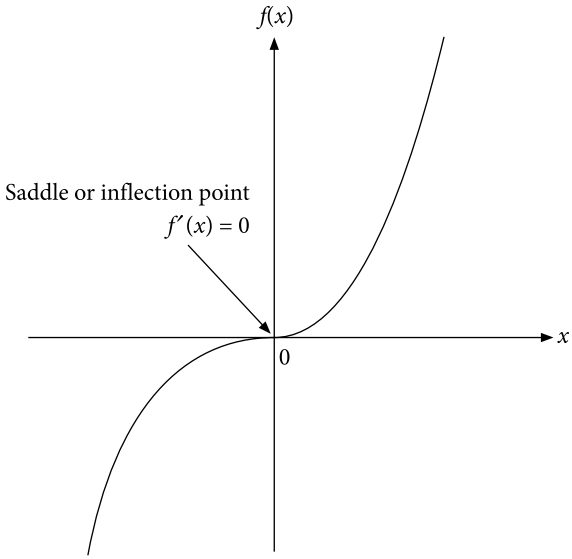

Fig. 3.3 Inflection or saddle point

Theorem 3.2

Sufficient Condition

We will apply the sufficient condition to get more idea about the stationary point.

Let $f'(x^*) = f''(x^*) = f'''(x^*) = \ldots\ldots\ldots\ldots = f^{(n-1)}(x^*) = 0$, however, $f^n(x^*) \neq 0$. Then, the point x^* gives

i. a minimum value of $f(x)$ when $f^n(x^*) > 0$ and n is even

ii. a maximum value of $f(x)$ when $f^n(x^*) < 0$ and n is even

iii. neither a minimum nor a maximum when n is odd

Proof

Taylor's theorem is applied with remainder after n terms, we can write

$$f\left(x^{*}+h\right)=f\left(x^{*}\right)+hf'\left(x^{*}\right)+\frac{h^{2}}{2!}f''\left(x^{*}\right)+\ldots\ldots+\frac{h^{n-1}}{(n-1)!}f^{(n-1)}\left(x^{*}\right)+\frac{h^{n}}{n!}f^{(n)}\left(x^{*}+\theta h\right)$$

$$\text{for}\quad 0<\theta<1 \qquad (3.11)$$

Since, $f'\left(x^{*}\right)=f''\left(x^{*}\right)=f'''\left(x^{*}\right)=\ldots\ldots\ldots\ldots=f^{(n-1)}\left(x^{*}\right)=0,$ Eq. (3.11) can be written as

$$f\left(x^{*}+h\right)-f\left(x^{*}\right)=\frac{h^{n}}{n!}f^{(n)}\left(x^{*}+\theta h\right) \qquad (3.12)$$

As, $f^{n}(x^{*})\neq 0$, there must have an interval around x^{*} at every point x of which the nth derivative $f^{n}(x)$ has the same sign, as of $f^{n}(x^{*})$. Therefore, $f^{(n)}\left(x^{*}+\theta h\right)$ has the sign of $f^{(n)}(x^{*})$ at every point $x^{*}+h$ of this interval. When n is even, $h^{n}/n!$ is positive irrespective of the sign of h whether it is positive or negative, and therefore, $f(x^{*}+h)-f(x^{*})$ will have the similar sign as that of $f^{(n)}(x^{*})$. Thus, x^{*} will be a relative maximum if $f^{(n)}(x^{*})$ is negative and a relative minimum if $f^{(n)}(x^{*})$ is positive. When n is odd, $h^{n}/n!$ changes its sign as the sign of h changes; for this reason the point x^{*} is neither a minimum nor a maximum. In this case, the point x^{*} is termed as *point of inflection* (see Fig. 3.3).

Example 3.1

Find all stationary points for the function (Eq. (3.13)), and then determine the maximum and minimum values of the function.

$$f(x)=5x^{6}-36x^{5}+\frac{165}{2}x^{4}-60x^{3}+36 \qquad (3.13)$$

Solution

Since, $f'(x)=30x^{5}-180x^{4}+330x^{3}-180x^{2}=30x^{2}(x-1)(x-2)(x-3)$

for finding stationary points $f'(x) = 0$

$$30x^{2}(x-1)(x-2)(x-3)=0$$

$$\Rightarrow x=0,1,2,3$$

Stationary points are $x = 0$, $x = 1$, $x = 2$, and $x = 3$

Now,

$$f''(x)=150x^{4}-720x^{3}+990x^{2}-360x$$

Table 3.1 Values of stationary points

Values of x^*	Values of $f(x^*)$	Values of $f''(x^*)$	Comments
0	36	0	we must investigate the next derivative
1	27.5	60	a relative minimum
2	44	–120	a relative maximum
3	5.5	540	a relative minimum

The third derivative of the function is

$$f'''(x) = 600x^3 - 2160x^2 + 1980x - 360$$

at $x = 0$, $f'''(x) = -360$

since $f'''(x) \neq 0$ at $x = 0$, and $n = 3$ is odd number; $x = 0$ is neither a minimum nor a maximum, and it is an inflection point.

Example 3.2

Find all local optima of the function

$$f(x) = x^{\frac{1}{3}}(x-1) \tag{3.14}$$

Solution

The first derivative of the function is

$$f'(x) = \frac{1}{3}x^{\frac{-2}{3}}.(x-1) + x^{\frac{1}{3}}.1$$

$$= \frac{x+1}{3x^{\frac{2}{3}}} + x^{\frac{1}{3}}$$

$$= \frac{1+4x}{3x^{\frac{2}{3}}}$$

Applying necessary condition, we have $f'(x^*) = 0$

Therefore, $x = 0$, and $x = -1/4$

When $x = 0$, the denominator is zero; at this point $f'(x)$ is not defined. This is a critical point.

Second derivative of the function is

$$f''(x) = -\frac{2}{9}x^{\frac{-5}{3}} + \frac{4}{9}x^{\frac{-2}{3}} \tag{3.15}$$

We cannot find the value of second derivative at point $x = -1/4$, therefore, it is difficult to say if the point is local maxima or local minima. This problem can be tackled by numerical optimization method.

3.2.2 Classification of unconstrained minimization methods

There are various techniques available for solving an unconstrained minimization problem. These techniques can be categorized into two broad classes such as direct search methods and descent methods. The direct search methods do not use the partial derivatives of the function; only the objective function values are require to find the minimum. Therefore, these methods are often called the non-gradient methods. As they utilize zeroth-order derivatives of the function, the direct search methods are also called zeroth-order methods. When the number of variables is relatively small, these methods are most suitable. In general, these methods are less effective than the descent methods. In addition to the function values, the descent methods require the first and in some instances the second derivatives of the objective function. Descent methods are usually more effective than direct search techniques as they use more information (through the use of derivatives) about the function for minimizing. The descent methods are also called gradient methods. Among these gradient methods, those utilizing only first derivatives of the function are known as first-order methods; those utilizing both first and second derivatives of the function are called second-order methods.

Unimodal function

A function is said to be an unimodal function when it consists of either one valley (minimum) or peak (maximum) only within the specified interval $[a, b]$. Therefore, a single-variable function is supposed to be unimodal when for any two specified points that lie on the same side of the optimum, the one that is closer to the optimum point gives the better value of the functional (smaller value for a minimization problem and larger value for a maximization problem). Mathematically this can be written as follows:

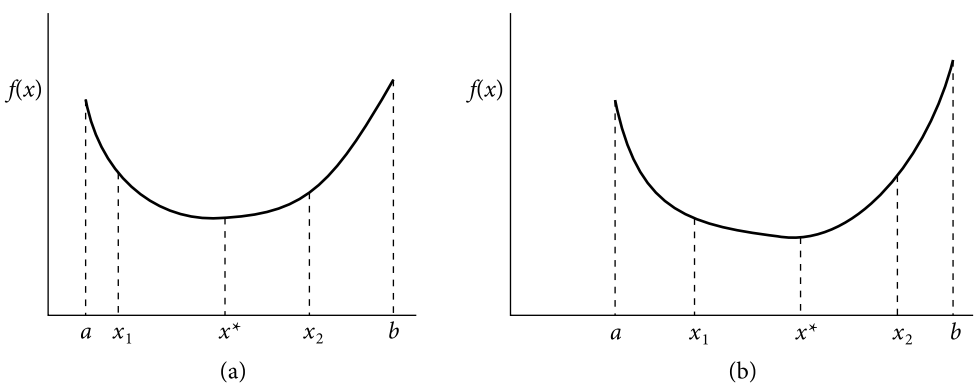

Fig. 3.4 Unimodal functions

Suppose $f(x)$ is strictly unimodal on the interval $a \le x \le b$ with a minimum at x^*. Let two points x_1 and x_2 be in the given interval such that $a < x_1 < x_2 < b$.

By comparing the values of the function at x_1 and x_2, the following conclusion can be drawn:

i. When $f(x_1) > f(x_2)$, then the minimum of $f(x)$ does not lie in the interval (a, x_1) or, $x^* \in (x_1, b)$ (see Fig. 3.4a).

ii. When $f(x_1) < f(x_2)$, then the minimum of $f(x)$ does not lie in the interval (x_2, b). In other words, $x^* \in (a, x_2)$ (see Fig. 3.4b).

Unimodality is a very significant functional property and almost all the search techniques currently in use for single-variable optimization require at least the assumption that the function is unimodal within the domain of interest. The usefulness of this characteristic lies in the fact that when $f(x)$ is unimodal we are required to compare $f(x)$ only at two different points for predicting in which of the subintervals defined by those two points the optimum does not lie.

3.3 Direct Search Methods

The search techniques, which find a single-variable optimum by successive elimination of subintervals to shrink the residual interval of search, are known as region elimination methods.

3.3.1 Finding a bracket for a minimum

Bracketing is significantly required for the optimization of a single-variable function when we have no idea about the range of the solution. Now we will discuss a methodical way of determining a range $a < x < b$ that contains a minimum of $f(x)$. This technique utilizes the slope $f'(x)$ to give us an indication whether the minimum lies to the right or left of an initial point x_0. When $f'(x_0)$ is positive then lower function values will be found for $x < x_0$, while $f'(x_0) < 0$ indicates lower values of $f(x)$ arise when $x > x_0$. Basically, the step size in this algorithm becomes larger and larger in a "downhill" direction until the function value starts to increase, which signifies that the minimum has been bracketed.

How to find a and b for bracketing a local minimum of f(x)

Select an initial point x_0 and a step length α (> 0)

Set $\delta = \text{sign}\left(f'(x_0)\right) \times [-\alpha]$

Repeat for i = 0, 1, 2, . . .

$x_{i+1} = x_i + \delta$, $\delta = 2\delta$

until $f(x_{i+1}) > f(x_i)$

if i = 0 then set $a = x_0$ and $b = x_1$

if $i > 0$ then set $a = x_{i-1}$ and $a = x_{i+1}$

3.3.2 Unrestricted search method

The optimum solution lies within the restricted ranges of design variables for most of the practical applications. In some instances, this range is unknown to us, and therefore, we need to perform the search procedure without any restrictions on the values of the variables.

Search with Fixed Step Size

This is the most straightforward method to solve a problem where we start moving from an initial guess point in a suitable direction (negative or positive) with a fixed step size. The size of the step used should be small in comparison to the desired final accuracy. Even though this process is very simple to execute, it is not effective in many situations. This process is explained by the following steps:

1. Start with x_1, an initial guess point.
2. Calculate $f_1 = f(x_1)$.
3. Consider a step size s, find $x_2 = x_1 + s$.
4. Calculate $f = f(x_2)$.
5. When the problem is of minimization one and if $f_2 < f_1$, from the assumption of unimodality we get the indication that the desired minimum cannot lie at $x < x_1$. Therefore, the search procedure required to continue further through the points x_3, x_4 ..... using the concept of unimodality while checking each pair of experiments. This search process is continued till the function value starts to increase at a point $x_i = x_1 + (i - 1)$.
6. The search process is terminated at point x_i, and either x_{i-1} or x_i is considered as the optimum point.
7. On the other hand, when $f_2 > f_1$, the search should be performed in the opposite direction at x_{-2}, x_{-3} ...,... points, where $x_{-j} = x - (j - 1)s$.
8. The desired minimum lies in between x_1 and x_2 when we get $f_2 = f_1$, and either x_1 or x_2 is considered as the minimum point. Sometimes we consider the middle point of $[x_1, x_2]$ as the minimum.
9. And when it occurs that f_{-2} and f_2 both are greater than f_1, it specifies that the desired minimum will lie in the double interval $x_{-2} < x < x_2$.

Search with Accelerated Step Size:

During the real life application, search with the fixed step size is very simple to execute. Despite this advantage, the major drawback arises owing to the unrestricted nature of the region within which the minimum is located. Sometimes, the number of iterations becomes very large. For example, when the optimum point of a specified function supposed to be at $x_{opt} = 10,000$ and, without proper information about the position of the minimum, if we arbitrarily select x_1 and s as 0.0 and 0.1, respectively, we are require to calculate the function value 1,000,001 times to locate the minimum point. This method is involved with a huge amount of computational work. If we gradually increase the step size till the minimum point is bracketed, an obvious improvement can be done. A very common practice is that of doubling the size of the step during search process as long as it shows an upgrading of the objective function. This method can be improved in different ways. One such option is that, after bracketing the optimum in (x_{i-1}, x_i), decrease the step length.

By starting the search process either from x_{i-1} or x_i, the fundamental method can be performed with a reduced step size. This search process is repeated until the interval that is bracketed turns into adequately small. The search process with accelerated step size can be demonstrated by the following example.

Example 3.3

Air is to be compressed from 1 to 10 atm. pressure in a two-stage compressor. To increase the compression efficiency, the compressed air from the first stage of compression is cooled (it is passed through a heat exchanger) before entering the second stage of compression. For isentropic compression of air the total work input to a compressor (W) can be represented by

$$W = c_p T_1 \left[\left(\frac{p_2}{p_1} \right)^{(k-1)/k} + \left(\frac{p_3}{p_2} \right)^{(k-1)/k} - 2 \right] \tag{3.16}$$

where the specific heat of air at constant pressure is c_p = 1.006 kJ/kg. K, k = 1.4 is the ratio of specific heat at constant pressure to specific heat at constant volume of air, and the entering gas temperature T_1 = 300K. Find the intermediate pressure p_2 at which cooling is required to minimize the work input to the compressor. Also, calculate the minimum work required to operate the compressor. Use search method with accelerated step size. Starting point = 1.0 (as the inlet pressure is 1 atm.) and initial step size = 0.05

Solution

Substituting the value of different parameters we get

$$W = 301.8 \left[\left(p_2 \right)^{0.286} + \left(\frac{10}{p_2} \right)^{0.286} - 2 \right] \tag{3.17}$$

We will start searching from the starting point = 1.0 (as the inlet pressure is 1 atm.) and with an initial step size = 0.05. The values of successive iterations are given in Table 3.2.

Table 3.2 Values of successive iterations with accelerated step size

i	Value of s	$x_i = x_1 + s$	$f_i = f(x_i)$	Is $f_i > f_{i-1}$?
1		1.0	281.27	--
2	0.05	1.05	277.43	No
3	0.1	1.1	273.93	No
4	0.2	1.2	267.80	No
5	0.4	1.4	258.26	No
6	0.8	1.8	246.29	No
7	1.6	2.6	236.69	No
8	3.2	4.2	238.14	Yes

Table 3.2 shows that the minimum point should be lie between 2.6 and 4.2. Figure 3.5 shows that minimum value is 3.15.

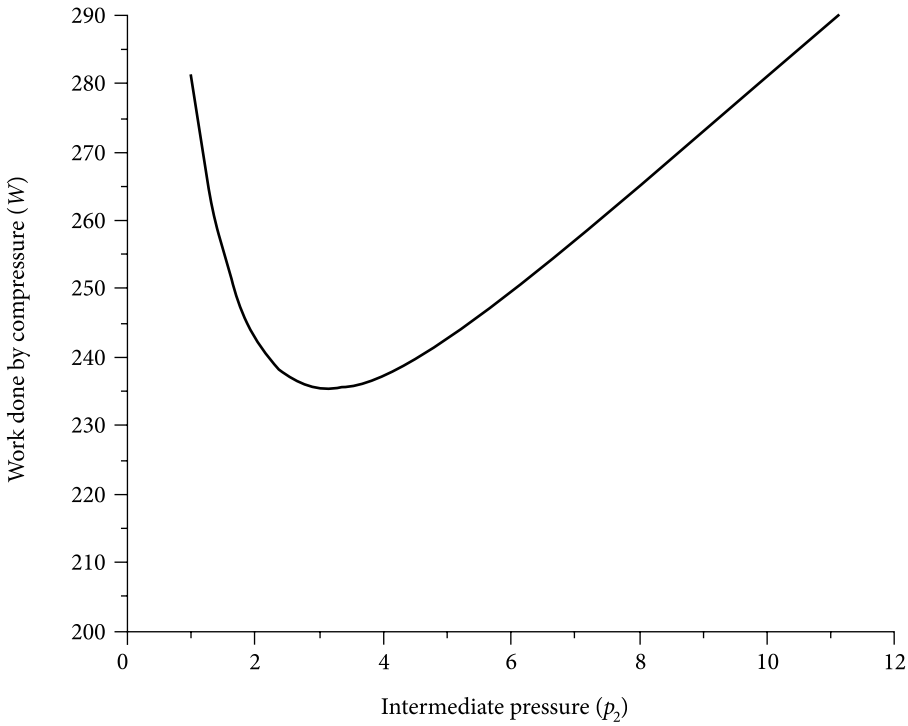

Fig. 3.5 Work done vs. intermediate pressure graph

3.3.3 Exhaustive search

In some search processes, we have plenty of knowledge about the region in which optimum is located. The exhaustive search technique can be applied for solving those problems wherever the interval in which the optimum point lies is finite. Suppose the starting and final points of the interval of uncertainty is represent by x_s and x_f respectively (see Fig. 3.6). The exhaustive search process includes the evaluation of the objective function at some equally spaced points within the interval (x_s, x_f). This number of points is predetermined by the user. Then reduce the interval of uncertainty by utilizing the concept of unimodality. Consider that the function (workdone by compressor) is defined on the interval (x_s, x_f). Eight equally spaced interior points $x_1 = 2$ to $x_8 = 9$ atm. pressure can be placed within this interval.

Considering that the values of the function are found as shown in Fig. 3.6, according to the assumption of unimodality, the minimum point must lie between points $x_2 = 3$ and $x_4 = 4$. Therefore, the interval (x_2, x_4) i.e., (3.0, 4.0) can be taken as the final interval of uncertainty. Generally, when the value of any function is calculated at n equally spaced points within the

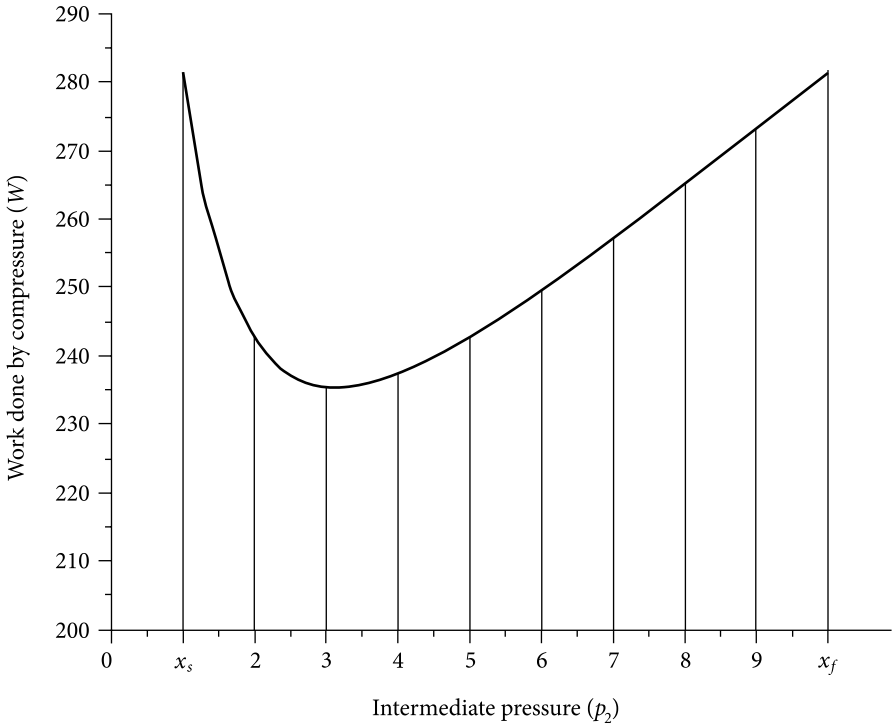

Fig. 3.6 Exhaustive search (see Example 3.3)

original interval of uncertainty of length $L_0 = x_f - x_s$, and if the point x_j shows the optimum value of the function (among these n values of the function), the final interval of uncertainty is given by

$$L_n = x_{j+1} - x_{j-1} = \frac{2}{n+1} L_0 \tag{3.18}$$

The final interval of uncertainty will change with the number of points. For various numbers of trial points in the exhaustive search method, the available final interval of uncertainty is given in Table 3.3:

Table 3.3 The available interval of uncertainty after different trials

Number of trials	2	3	4	5	6	…	n
L_n/L_0	2/4	2/4	2/5	2/6	2/7	…	$2/(n+1)$

This method is known as simultaneous search method since the function value is calculated at all n points simultaneously. Whereas, in sequential search methods the information obtained from the initial trials is utilized to place the subsequent experiments. The sequential search methods are relatively more efficient compared to the simultaneous search.

Example 3.4

Solve the Example 3.3 by exhaustive search method. Maximum error should be less than 10 per cent.

Solution

The middle point of the final interval of uncertainty is considered as the approximate optimum point, and then the maximum deviation will be $1/(n+1)$ times the initial interval of uncertainty. Hence, to estimate the optimum within 10 per cent of the exact value, we have

$$\frac{1}{n+1} \leq \frac{1}{10} \text{ or } n \geq 9$$

We use Eq. (3.17) as the function that is to be minimize by considering $n = 9$, the following function values have been found out:

Table 3.4 Work done with different intermediate pressure (Exhaustive search method)

i	1	2	3	4	5	6	7	8	9
p_2	2	3	4	5	6	7	8	9	10
W	242.59	235.47	237.27	242.59	249.50	257.13	265.11	273.19	281.27

Table 3.4 shows that the optimum point should lay in between 3 and 4.

3.3.4 Dichotomous search

In exhaustive search method, we need to perform all the experiments simultaneously before taking any decision regarding the position of the optimum point. Unlike the exhaustive search method, dichotomous search method, interval halving method, Fibonacci method and the golden section method discussed in the following sections, are all sequential search methods. The experiments are placed sequentially for these methods. In these methods, the position of the any experiment is influenced by the outcome of previous experiment. During this dichotomous search process, two experiments are performed very close to the center of the interval of uncertainty. As the points very close to the centre, almost half of the interval of uncertainty is eliminated depending on the relative values of the objective function at those two points. The locations of these two experiments are estimated by the following equations.

$$x_1 = \frac{L_0}{2} - \frac{\delta}{2} \tag{3.19}$$

$$x_2 = \frac{L_0}{2} + \frac{\delta}{2} \tag{3.20}$$

where δ is a small positive number. We have to chose the value of δ in such a way that the result of two experiments will be significantly different. After the first experiment, the new interval of

uncertainty can be represented by $(L_0/2 + \delta/2)$. The process of dichotomous search works based on the performing a pair of experiments near the center of the existing interval of uncertainty. Therefore, the next pair of experiments is performed near the center of the residual interval of uncertainty. By this method, the interval of uncertainty becomes almost half after each pair of experiment. The following table shows the intervals of uncertainty at the end of different pairs of experiments:

Table 3.5 Final intervals of uncertainty for different pairs of experiments

Number of experiments	2	4	6
Final interval of uncertainty	$\frac{1}{2}(L_0 + \delta)$	$\frac{1}{2}\left(\frac{L_0 + \delta}{2}\right) + \frac{\delta}{2}$	$\frac{1}{2}\left(\frac{L_0 + \delta}{4} + \frac{\delta}{2}\right) + \frac{\delta}{2}$

usually, the final interval of uncertainty after performing n experiments (where n is an even number) is given by

$$L_n = \frac{L_0}{2^{n/2}} + \delta\left(1 - \frac{1}{2^{n/2}}\right) \tag{3.21}$$

The Example 3.5 is given to demonstrate this search method.

Example 3.5

Solve the problem given in Example 3.3 by dichotomous search method. Maximum error should be less than 10 per cent.

Solution

We can write the ratio of final to initial intervals of uncertainty by using Eq. (3.21).

$$\frac{L_n}{L_0} = \frac{1}{2^{n/2}} + \frac{\delta}{L_0}\left(1 - \frac{1}{2^{n/2}}\right) \tag{3.22}$$

where δ is a very small quantity, say 0.001, and n is the number of experiments. If we consider the middle point of the final interval as the desired optimum point, the requirement can be stated as

$$\frac{1}{2}\frac{L_n}{L_0} \le \frac{1}{10}$$

$$\frac{1}{2^{n/2}} + \frac{\delta}{L_0}\left(1 - \frac{1}{2^{n/2}}\right) \le \frac{1}{5}$$

Since, $\delta = 0.001$ and $L_0 = 9$, we have

$$\frac{1}{2^{n/2}} + \frac{0.001}{9}\left(1 - \frac{1}{2^{n/2}}\right) \leq \frac{1}{5}$$

$$\frac{1}{2^{n/2}} + \frac{1}{1111}\left(1 - \frac{1}{2^{n/2}}\right) \leq \frac{1}{5}$$

$$\frac{1110}{1111}\frac{1}{2^{n/2}} \leq \frac{1106}{5555}$$

$$2^{n/2} \geq \frac{5550}{1106} \simeq 5.0$$

As we are performing two experiments each time, the n should to be even. From the above inequality, we get the minimum acceptable value of $n = 6$.

The search process is performed as follows. The first two experiments are conducted at

$$x_1 = \frac{L_0}{2} - \frac{\delta}{2} = 4.5 - 0.0005 = 4.4995$$

$$x_2 = \frac{L_0}{2} + \frac{\delta}{2} = 4.5 + 0.0005 = 4.5005$$

the function values at these points are given by

$$f_1 = f(x_1) = 239.6468$$

$$f_2 = f(x_2) = 239.6522$$

Since, $f_2 > f_1$, the new interval of uncertainty will be (1.0, 4.4995). The second pair of experiments is carried out at

$$x_3 = \frac{3.4995}{2} - \frac{0.001}{2} = 1.7498 - 0.0005 = 1.7493$$

$$x_4 = \frac{3.4995}{2} + \frac{0.001}{2} = 1.7498 + 0.0005 = 1.7503$$

the function values are calculated as follows

$$f_3 = f\left(x_3\right) = 247.4326$$

$$f_4 = f\left(x_4\right) = 247.4092$$

Since, $f_3 > f_4$, the new interval of uncertainty will be (1.7493, 4.4995).

The final set of experiments are performed at

$$x_5 = 1.7493 + \frac{2.7502}{2} - \frac{0.001}{2} = 1.7493 + 1.3751 - 0.0005 = 3.1239$$

$$x_6 = 1.7493 + \frac{2.7502}{2} + \frac{0.001}{2} = 1.7493 + 1.3751 + 0.0005 = 3.1249$$

The corresponding values of the function are

$$f_5 = f\left(x_5\right) = 235.3805$$

$$f_6 = f\left(x_6\right) = 235.3803$$

Since, $f_5 > f_6$, then the new interval of uncertainty is (3.1249,4.4995). The middle point of this interval is considered as optimum point, and therefore,

$$x_{\text{opt}} \simeq 3.8122 \text{ and } f_{\text{opt}} \simeq 236.5745$$

3.3.5 Interval halving method

Interval halving method is a very useful and simple search method. In every stage of this method, exactly one-half of the current interval of uncertainty is eliminated. In the first stage of this process, three experiments are needed and two experiments in each succeeding stage. Because, in all the stages except the first stage of this process, value of the function will be available at the middle point of the interval of uncertainty (f_0). This method can be illustrated by the following steps:

Step 1 Split $L_0 = [a, b]$, the initial interval of uncertainty into four equal parts. The point x_0 is labeled as the middle point and the quarter-interval points x_1 and x_2 as shown in Fig. 3.7.

Step 2 The value of the function $f(x)$ has been calculated at these three interior points to get $f = f(x_1)$, $f_0 = f(x_0)$, and $f_2 = f(x_2)$.

Step 3 (a) When $f_2 > f_0 > f_1$, discard the interval (x_0, b), label x_1 and x_0 as the new x_0 and b, respectively, and move to step 4.

(b) If $f_2 < f_0 < f_1$, remove the interval (a, x_0), label x_0 and x_2 as the new a and x_0, respectively, and move to step 4.

(c) When $f_1 > f_0$ and $f_2 > f_0$, remove both the intervals (a, x_1) and (x_2, b), then label x_1 as new a and x_2 as new b, and move to step 4.

Step 4 Check whether $L = b - a$, the new interval of uncertainty, satisfies the convergence criterion $L \leq \varepsilon$, where ε is considered as a small quantity. Stop the process when it satisfies the convergence criterion. Or else, set the new $L_0 = L$ and go to step 1.

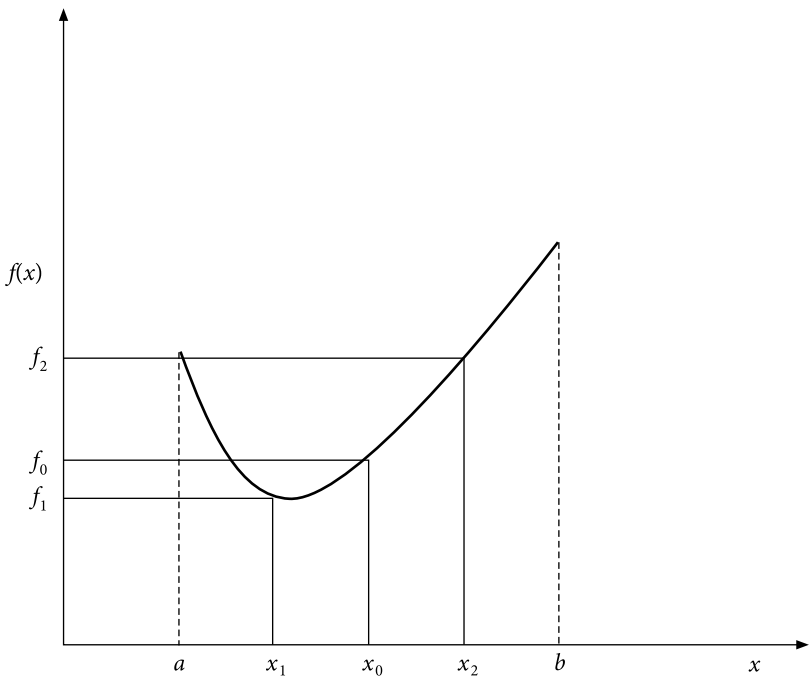

Fig. 3.7 Interval halving method

After the completion of n experiments ($n \geq 3$ and odd), the interval of uncertainty left over can be represented by

$$L_n = \left(\frac{1}{2}\right)^{(n-1)/2} L_0 \tag{3.23}$$

Example 3.6

Solve the Example 3.3 by interval halving method. Maximum error should be less than 10 per cent.

Solution

If we consider that the optimum point will be located at the middle point of the final interval of uncertainty, the required accuracy level can be reached when

$$\frac{1}{2}L_n \le \frac{L_0}{10} \text{ or } \left(\frac{1}{2}\right)^{(n-1)/2} L_0 \le \frac{L_0}{5}$$

for $L_0 = 9$, we have

$$\left(\frac{1}{2^{(n-1)/2}}\right) \le \frac{1}{5} \text{ or } 2^{(n-1)/2} \ge 5$$

Since, n should to be odd number, the above inequality provides us the minimum acceptable value of n as 7. Considering the value of $n = 7$, the search process is carried out as follows. The first three experiments are placed at one-fourth, middle, and three-fourth points of the interval $L_0 = [a = 1, b = 10]$ as

$$x_1 = 3.25, \; f_1 = 235.4011$$

$$x_0 = 5.50, \; f_0 = 245.9077$$

$$x_2 = 7.75, \; f_2 = 263.0979$$

Since, $f_2 > f_0 > f_1$, we eliminate the interval $(x_0, b) = (5.50, 10.00)$, new $a = 1.00$ and $b = 5.50$ By dividing the new interval of uncertainty, $L_3 = [1.00, 5.50]$ into four equal parts, we have

$$x_1 = 2.125, \; f_1 = 240.8034$$

$$x_0 = 3.25, \; f_0 = 235.4011$$

$$x_2 = 4.375, \; f_2 = 238.9937$$

Since, $f_1 > f_0$ and $f_2 > f_0$, we remove both the intervals (a, x_1) and (x_2, b). Now the new interval is $L_5 = [a = 2.125, b = 4.375]$. This interval is again divided into four equal parts to obtain

$$x_1 = 2.6875, \; f_1 = 236.2837$$

$$x_0 = 3.25, \; f_0 = 235.4011$$

$$x_2 = 3.8125, \; f_2 = 236.5755$$

In this experiment we notice that $f_1 > f_0$ and $f_2 > f_0$ therefore, we remove both the intervals (a, x_1) and (x_2, b) to get the new interval of uncertainty as $L_7 = (2.6875, 3.8125)$. Considering the middle point of this interval as optimum, we have

$$x_{\text{opt}} \simeq 3.25 \text{ and } f_{\text{opt}} \simeq 235.4011$$

3.3.6 Fibonacci method

The Fibonacci method is useful to find the minimum of a single variable function. This method can be applied even if the function is not continuous. Despite many advantages, Fibonacci method has some limitations like other elimination methods:

i. This is not a global search method. We should know the initial interval of uncertainty within which the optimum is located.

ii. The objective function being optimized should be unimodal within the initial interval of uncertainty.

iii. We are not able to locate the exact value of optimum by using this method. Only an interval will be estimated; this interval is known as the final interval of uncertainty. The length of the final interval of uncertainty can be controlled. This interval can be found as small as we require by increasing the computational effort.

iv. In this method, we need to specify the number of function evaluations to be made in the search process or we have to specify the required level of resolution.

This search process uses of the sequence of Fibonacci numbers $\{F_n\}$, for conducting the experiments. These numbers can be defined as

$$F_0 = F_1 = 1 \tag{3.24}$$

$$F_n = F_{n-1} + F_{n-2},\ n = 2, 3, 4 \ldots \tag{3.25}$$

which gives us the sequence 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, …

Algorithm

Suppose the initial interval of uncertainty L_0 is defined by $a \le x \le b$ and n is the total number of experiments to be carried out. We can define

$$L_2^* = \frac{F_{n-2}}{F_n} L_0 \tag{3.26}$$

and locate the points x_1 and x_2 for the first two experiments. These points are placed at a distance of L_2^* from each end of L_0. Which yield

$$x_1 = a + L_2^* = a + \frac{F_{n-2}}{F_n} L_0 \tag{3.27}$$

$$x_2 = b - L_2^* = b - \frac{F_{n-2}}{F_n} L_0 = a + \frac{F_{n-1}}{F_n} L_0 \tag{3.28}$$

By using the unimodality assumption, remove one part of the interval. Then the remaining part is a smaller interval of uncertainty L_2 that can be written as

$$L_2 = L_0 - L_2^* = L_0\left(1 - \frac{F_{n-2}}{F_n}\right) = \frac{F_{n-1}}{F_n}L_0 \tag{3.29}$$

and there is one experiment left in this search process. This experiment is placed at a distance of

$$L_2^* = L_0\frac{F_{n-2}}{F_n} = L_2\frac{F_{n-2}}{F_{n-1}} \tag{3.30}$$

from one end and

$$L_2 - L_2^* = L_0\frac{F_{n-3}}{F_n} = L_2\frac{F_{n-3}}{F_{n-1}} \tag{3.31}$$

from the other end. The 3rd experiment is now placed in the interval L_2 such a way that the current two experiments are positioned at a distance of

$$L_3^* = L_0\frac{F_{n-3}}{F_n} = L_2\frac{F_{n-3}}{F_{n-1}} \tag{3.32}$$

from each end of the interval L_2. Again, we can reduce the interval of uncertainty to L_3 by using the unimodality property. The value of L_3 is represented by

$$L_3 = L_2 - L_3^* = L_2 - L_2\frac{F_{n-3}}{F_{n-1}} = L_2\frac{F_{n-2}}{F_{n-1}} = L_0\frac{F_{n-2}}{F_n} \tag{3.33}$$

We can continue the process of eliminating a certain interval and conducting a new experiment in the residual interval. The position of the jth experiment and the interval of uncertainty at the completion of j experiments are given by Eq. (3.34) and Eq. (3.35) respectively.

$$L_j^* = L_{j-1}\frac{F_{n-j}}{F_{n-(j-2)}} \tag{3.34}$$

$$L_j = L_0\frac{F_{n-(j-1)}}{F_n} \tag{3.35}$$

For a n predetermined experiments, the ratio of the interval of uncertainty remaining after performing j experiments to the initial interval of uncertainty becomes

$$\frac{L_j}{L_0} = \frac{F_{n-(j-1)}}{F_n} \tag{3.36}$$

and when $j = n$, we have

$$\frac{L_n}{L_0} = \frac{F_1}{F_n} = \frac{1}{F_n} \tag{3.37}$$

The ratio L_n/L_0 will allow us to estimate the value of n, the number of experiments needed to reach the optimum point with any desired level of accuracy.

Example 3.7

Solve the problem given in Example 3.3 using Fibonacci method taking $n = 6$.

Solution

The given value of $n = 6$ and $L_0 = 9.00$, which yield

$$L_2^* = L_0 \frac{F_{n-2}}{F_n} = (9.00)\frac{5}{13} = 3.4615385$$

hence, the locations of the first two experiments are given by

$$x_1 = 1.00 + 3.4615385 = 4.4615385, \quad f_1 = 239.4438353$$

$$x_2 = 9.00 - 3.4615385 = 5.5384615, \quad f_2 = 246.1751813$$

Since, $f_1 < f_2$, we can remove the interval $[x_2, 9.00]$ by using the assumption of unimodality.

Placing the third experiment at

$$x_3 = 1.00 + (5.5384615 - 4.4615385) = 2.076923$$

the corresponding function value is

$$f_3 = 241.4471087$$

Since, $f_1 < f_3$, we eliminate the interval $[x_3, 1.00]$. The new interval is $[x_3, x_2]$.

The next experiment is placed at $x_4 = 3.153846$ with $f_4 = 235.3756528$

Here, $f_4 < f_1$, therefore, we remove the interval $[x_1, x_2]$. The position of the next experiment can be found as $x_5 = 3.3846155$, and the corresponding objective function value of $f_5 = 235.5338301$.

Since, $f_4 < f_5$, we eliminate the interval $[x_5, x_1]$. The new interval is $[x_3, x_5] = [2.076923, 3.3846155]$

The final experiment is positioned at $x_6 = 2.3076925$ with the corresponding objective function value of $f_6 = 238.7833231$.

Since, $f_4 < f_6$, we remove the interval $[x_3, x_6]$. The new interval is $[x_6, x_5] = [2.3076925, 3.3846155]$

Considering the middle point as the optimum point

$$x_{\text{opt}} \simeq 2.846154 \text{ and } f_{\text{opt}} \simeq 235.7560691$$

3.3.7 Golden section method

The golden section method is also a search technique similar to the Fibonacci method. The main dissimilarity is that the total number of experiments to be performed in the Fibonacci method is required to mention before starting the calculation, while this is not necessary in the golden section method. In the Fibonacci method, the total number of experiments (N) determines the location of the first two experiments. We start the golden section method with a presumption that we are ready to perform a quite large number of experiments. However, we are able to decide the total number of experiments during the computation. After completion of the various numbers of experiments, the intervals of uncertainty can be calculated as follows:

$$L_2 = \lim_{N\to\infty} \frac{F_{N-1}}{F_N} L_0 \tag{3.38}$$

$$L_3 = \lim_{N\to\infty} \frac{F_{N-2}}{F_N} L_0 = \lim_{N\to\infty} \frac{F_{N-2}}{F_{N-1}} \frac{F_{N-1}}{F_N} L_0 \tag{3.39}$$

$$\simeq \lim_{N\to\infty} \left(\frac{F_{N-1}}{F_N} \right)^2 L_0 \tag{3.40}$$

We can generalize this result to obtain

$$L_k = \lim_{N\to\infty} \left(\frac{F_{N-1}}{F_N} \right)^{k-1} L_0 \tag{3.41}$$

Using the relation

$$F_N = F_{N-1} + F_{N-2} \tag{3.42}$$

after dividing both sides of the above equation by F_{N-1} we obtain

$$\frac{F_N}{F_{N-1}} = 1 + \frac{F_{N-2}}{F_{N-1}} \tag{3.43}$$

By defining a ratio γ as

$$\gamma = \lim_{N\to\infty}\left(\frac{F_N}{F_{N-1}}\right) \tag{3.44}$$

Equation (3.43) can be expressed as

$$\gamma \simeq \frac{1}{\gamma} + 1 \tag{3.45}$$

that is,

$$\gamma^2 - \gamma - 1 = 0 \tag{3.46}$$

This gives the root $\gamma = 1.618$, and hence, Eq. (3.41) yields

$$L_k = \left(\frac{1}{\gamma}\right)^{k-1} L_0 = (0.618)^{k-1} L_0 \tag{3.47}$$

For large values of N, the ratios F_{N-2}/F_{N-1} and F_{N-1}/F_N in Eq. (3.40) have been taken to be same. The following table (Table 3.6) confirms the validity of this assumption:

Table 3.6 Final interval of uncertainty by golden section method

Value of *N*	2	3	4	5	6	7	8	9	10	∞
Ratio $\frac{F_{N-1}}{F_N}$	0.5	0.667	0.6	0.625	0.6156	0.619	0.6177	0.6181	0.6184	0.618

The term golden section is very old and it is found in the Euclidean geometry. According to Euclid's geometry, if we split a line segment into two unequal parts so that the ratio of the whole to the larger part is equal to the ratio of the larger to the smaller, the division is called the golden section and the ratio is called the golden mean.

Algorithm

The algorithm of golden section method is similar to the Fibonacci method except that the position of the first two experiments is given by

$$L_2^* = \frac{F_{N-2}}{F_N} L_0 = \frac{F_{N-2}}{F_{N-1}} \frac{F_{N-1}}{F_N} L_0 = \frac{L_0}{\gamma^2} = 0.382 L_0 \tag{3.48}$$

For stopping the process, the required accuracy level can be specified.

Example 3.8

Solve the Example 3.3 by golden section method using $n = 6$.

Solution

The first two experiments are placed according to the following calculation

$$L_2^* = 0.382 L_0 = (0.382)(9.00) = 3.438$$

thus, $x_1 = 4.438$ and $x_2 = 5.562$ with $f_1 = 239.3196483$ and $f_2 = 246.3396105$

Since, $f_1 < f_2$, we remove the interval $[x_2, 9.00]$ based on the unimodality assumption and get the new interval of uncertainty as $L_2 = [1.00, x_2] = [1.00, 5.562]$.

The third experiment is positioned at

$$x_3 = 1.00 + (x_2 - x_1) = 2.124 \text{ and } f_3 = 240.8162691$$

Since, $f_3 > f_1$, we can delete the interval $[x_1, x_2]$ and get a new interval of uncertainty as $[1.00, x_1] = [1.00, 4.438]$

The location of the next experiment is given by

$$x_4 = 3.314 \text{ and } f_4 = 235.4507654$$

Since, $f_3 > f_4$, we can delete the interval $[1.00, x_3]$ and a new interval of uncertainty as $[x_3, x_1] = [2.124, 4.438]$ is obtained.

The next experiment is positioned at

$$x_5 = 3.248 \text{ and function value } f_5 = 235.3999553$$

Since, $f_4 > f_5$, we can delete the interval $[x_4, x_1]$ and obtain a new interval of uncertainty as $[x_3, x_4] = [2.124, 3.314]$

The final experiment is placed at

$x_6 = 2.190$ and corresponding function value $f = 240.0110286$

Since, $f_6 > f_5$, we can remove the interval $[x_3, x_6]$ and obtain a new interval of uncertainty as $[x_6, x_4] = [2.190, 3.314]$.

If we consider the middle point of the final interval as optimum point, we have

$$x_{opt} \simeq 2.752 \text{ and } f_{opt} \simeq 236.0381082$$

3.4 Direct Root Methods

The necessary condition for $f(x)$ to possesses a minimum at the point x^* is that $f'(x^*) = 0$. In the direct root methods, we will try to find the solution (or roots) of the equation $f'(x) = 0$. In this

section, we have discussed three root-finding methods namely, the Newton, the Quasi-Newton, and the secant methods.

3.4.1 Newton method

Originally the Newton method was proposed by Newton to solve nonlinear equations and afterward it is modified by Raphson, therefore, this method is also familiar as Newton–Raphson method in the field of numerical analysis.

Consider the quadratic approximation of the function $f(x)$ at $x = x_i$ using the Taylor's series expansion

$$f(x) = f(x_i) + f'(x_i)(x - x_i) + \frac{1}{2} f''(x_i)(x - x_i)^2 \tag{3.49}$$

For the minimum of $f(x)$, we set the value of the derivative in Eq. (3.49) equal to zero, then we get

$$f'(x) = f'(x_i) + f''(x_i)(x - x_i) = 0 \tag{3.50}$$

If the point x_i represents an approximation to the minimum of $f(x)$, Eq. (3.50) is rearranged to achieve an improved approximation as

$$x_{i+1} = x_i - \frac{f'(x_i)}{f''(x_i)} \tag{3.51}$$

Therefore, the Newton method as represented by Eq. (3.51) is similar as the utilization of quadratic approximation for the function $f(x)$ and applying the necessary conditions. This iterative process shown in Eq. (3.51) can be assumed to have converged whenever the value of the derivative, $f'(x_{i+1})$, is close to zero:

$$\left| f'(x_{i+1}) \right| \leq \varepsilon \tag{3.52}$$

where ε is a small quantity. Figure 3.8 graphically explains the convergence process of the Newton method.

Notes

1. Both the first- and second-order derivatives of the function $f(x)$ have been used in this method.
2. When $f''(x_i) \neq 0$ [in Eq. (3.51)], the Newton iterative method possesses a very fast convergence property that is known as quadratic convergence.
3. When starting point is very close to the optimum point, Newton's method is suitable for that problem. The Newton iterative process might diverge when the starting point for the iterative process is far from the true solution x^*.

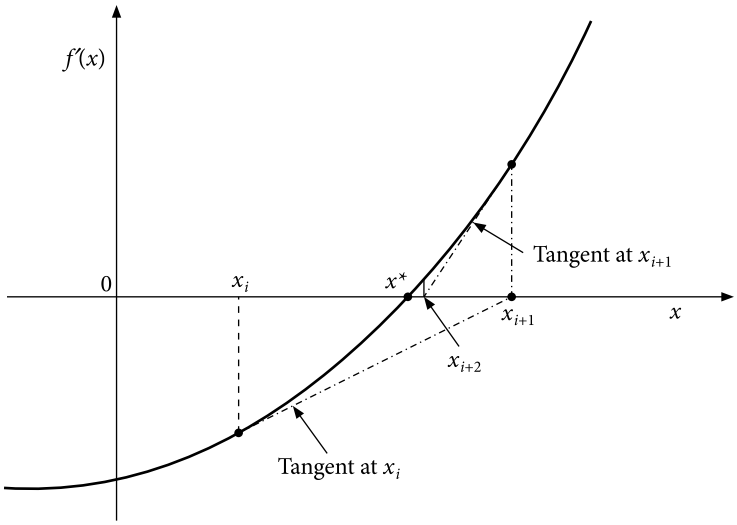

Fig. 3.8 Convergence process of Newton method

3.4.2 Quasi-Newton method

When the function $f(x)$ being minimized is not available in closed form or differentiation is also difficult, the derivatives $f'(x)$ and $f''(x)$ in Eq. (3.51) can be approximated using the finite difference formulas as

$$f'(x_i) = \frac{f(x_i + \Delta x) - f(x_i - \Delta x)}{2\Delta x} \tag{3.53}$$

$$f''(x_i) = \frac{f(x_i + \Delta x) - 2f(x_i) + f(x_i - \Delta x)}{\Delta x^2} \tag{3.54}$$

where Δx is a small step size. Substitution of Eqs (3.53) and (3.54) into Eq. (3.51) leads to

$$x_{i+1} = x_i - \frac{\Delta x\left[f(x_i + \Delta x) - f(x_i - \Delta x)\right]}{2\left[f(x_i + \Delta x) - 2f(x_i) + f(x_i - \Delta x)\right]} \tag{3.55}$$

The iterative process described by Eq. (3.55) is known as the Quasi-Newton method.

To check the convergence of this iterative process, the criterion given by Eq. (3.56) can be utilized:

$$\left|f'(x_{i+1})\right| = \left|\frac{f(x_{i+1} + \Delta x) - f(x_{i+1} - \Delta x)}{2\Delta x}\right| \le \varepsilon \tag{3.56}$$

where ε is a very small quantity and a central difference formula has been utilized for calculating the derivative of f.

Notes

1. Equations (3.55) and (3.56) have been developed by using the central difference formulas. We can also utilize the forward or backward difference formulas for the same.
2. In each iteration, Eq. (3.55) requires the estimation of the function at the points $x_i + \Delta x$ and $x_i - \Delta x$ in addition to x_i.

3.4.3 Secant method

An equation similar to Eq. (3.50) is employed to the secant method

$$f'(x) = f'(x_i) + s(x - x_i) = 0 \tag{3.57}$$

where s is the slope of the line that connects the two points $(a, f'(a))$ and $(b, f'(b))$, where a and b represent two different approximations to the actual solution, x^*. From Fig. 3.9, we can define the slope s as

$$s = \frac{f'(b) - f'(a)}{b - a} \tag{3.58}$$

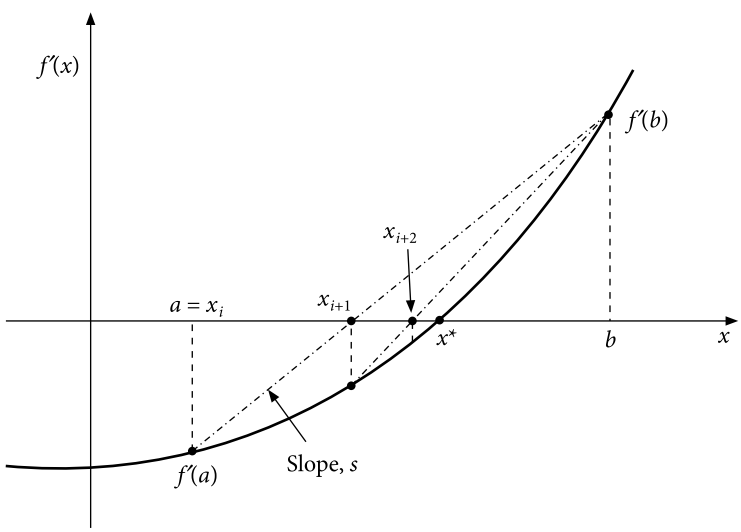

Fig. 3.9 Convergence process of secant method

Equation (3.57) approximates the function $f'(x)$ as a linear equation (secant) between the points a and b, and consequently the solution of Eq. (3.57) gives the new approximation to the root of $f'(x)$ as

$$x_{i+1} = x_i - \frac{f'(x_i)}{s} = a - \frac{f'(a)(b-a)}{f'(b) - f'(a)} \tag{3.59}$$

The iterative process expressed by the Eq. (3.59) is called the secant method (Fig. 3.9). The secant method can also be considered as a Quasi-Newton method as the secant approaches the second derivative of $f(x)$ at a as b approaches a. This method can also be considered as a form of elimination process as part of the interval (a, a_{i+1}) is eliminated in every iteration as shown in Fig. 3.9. The iterative process can be executed by using the following steps [Rao (2009)].

Step 1 Set $x_i = a = 0$ and calculate $f'(a)$. The value of $f'(a)$ will be negative. Assume an initial trial step length t_0. Set $i = 1$.

Step 2 Calculate $f'(t_0)$.

Step 3 If $f'(t_0) < 0$, set $a = x_i = t_0, f'(a) = f'(t_0)$ new $t_0 = 2t_0$, and go to step 2.

Step 4 If $f'(t_0) \geq 0$, set $b = t_0$, $f'(b) = f'(t_0)$, and move to step 5.

Step 5 The new approximate solution of the problem can be found as

$$x_{i+1} = a - \frac{f'(a)(b-a)}{f'(b) - f'(a)} \tag{3.60}$$

Step 6 Check the convergence criteria:

$$\left| f'(x_i + 1) \right| \leq \varepsilon$$

where ε is a small quantity. If the above convergence criteria is satisfied, consider $x^* \approx x_{i+1}$ as the solution and terminate the process. If not, move to step 7.

Step 7 If $f'(x_{i+1}) \geq 0$, set new $b = x_{i+1}, f'(b) = f'(x_{i+1})$, $i = i + 1$, and go to step 5.

Step 8 If $f'(x_{i+1}) < 0$, set new $a = x_{i+1}, f'(a) = f'(x_{i+1})$, $i = i + 1$, and go to step 5.

Comments

1. The secant method is the same as to considering a linear equation for $f'(x)$. This shows that the original function $f(x)$ is approximated by a quadratic equation.
2. In some cases we may come across the condition that the function $f'(x)$ varies very slowly with x. In this condition, we can identify it by observing that the point b remains unchanged for several consecutive iterations. When this situation is suspected, we can improve the convergence process by taking the next value of x_{i+1} as $(a + b)/2$ in place of finding its value from Eq. (3.60).

3.5 Polynomial Approximation Methods

There is another class of unidimensional minimization methods which locates a point x near x^* by interpolation and extrapolation using polynomial approximations as models of $f(x)$. This x is the value of the independent variable that corresponds to the minimum of $f(x)$. Both quadratic and

cubic approximation have been proposed in this section. We are using only the function values and using both function and derivative values for quadratic and cubic approximation respectively. These approximation methods have higher efficiency than other methods for those functions where $f'(x)$ is continuous. These methods are extensively used to perform line searches for finding the multivariable optimizers.

3.5.1 Quadratic interpolation

The quadratic interpolation method starts with three points x_1, x_2 and x_3 in increasing order that might be placed in equal distance, however, the extreme points (x_1 and x_3) must bracket the minimum. It is known to us that a quadratic function $f(x) = a + bx + cx_2$ can be passed exactly through the three points, and that the differentiation of the function can be estimated to find the minimum of the approximating function, the derivative of the function should be equal to 0. Then by solving $f'(x) = 0$, we get

$$\tilde{x} = -\frac{b}{2c} \tag{3.61}$$

consider that $f(x)$ is evaluated at x_1, x_2, and x_3, to find $f(x_1) = f_1$, $f(x_2) \equiv f_2$, and $f(x_3) \equiv f_3$. Now, we have three linear Eqs (3.62), (3.63), and (3.64) with three unknown variables. The coefficients a, b and c can be calculated from the solution of these three linear equations

$$f\left(x_1\right) = a + bx_1 + cx_1^2 \tag{3.62}$$

$$f\left(x_2\right) = a + bx_2 + cx_2^2 \tag{3.63}$$

$$f\left(x_3\right) = a + bx_3 + cx_3^2 \tag{3.64}$$

by means of determinants or matrix algebra. Incorporating the values of b and c expressed in terms of x_1, x_2, x_3, f_1, f_2 and f_3 into the Eq. (3.61) yields

$$\tilde{x}^* = \frac{1}{2}\left[\frac{\left(x_2^2 - x_3^2\right)f_1 + \left(x_3^2 - x_1^2\right)f_2 + \left(x_1^2 - x_2^2\right)f_3}{\left(x_2 - x_3\right)f_1 + \left(x_3 - x_1\right)f_2 + \left(x_1 - x_2\right)f_3}\right] \tag{3.65}$$

To demonstrate the first stage of this search process, examine the four points in Fig. 3.10. We are interested to reduce the initial interval $[x_1, x_3]$. We assume that the function $f(x)$ is unimodal and has a minimum. Then by examining the values of $f(x)$, we can eliminate the interval from x_1 to x_2, and utilize the region $[x_2, x_3]$ as the new interval. This new interval contains three points, $\left(x_2, \tilde{x}, x_3\right)$ that can be utilized to estimate a x^* value from the Eq. (3.65), and so on. Usually, we evaluate $f(x^*)$ and remove from the set $\{x_1, x_2, x_3\}$ the point that corresponds to the highest value of the function $f(x)$, unless a bracket on the minimum of $f(x)$ is lost by doing this, in which case we remove the x so as to maintain the bracket.

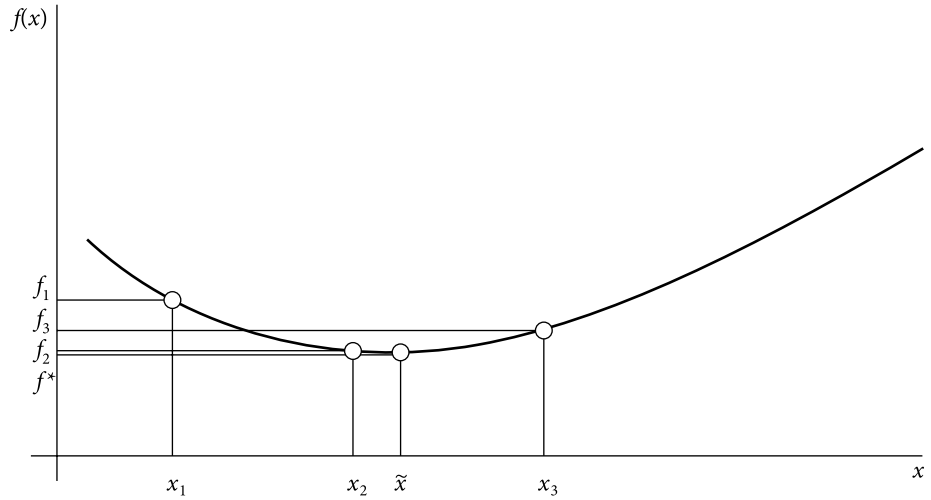

Fig. 3.10 Quadratic interpolation

3.5.2 Cubic interpolation

Cubic interpolation is used to find the minimum of $f(x)$ based on approximating the objective function by a polynomial of third degree within the interval of interest. After that, we determine the associated stationary point of the polynomial (3.66)

$$f(x) = a_1 x^3 + a_2 x^2 + a_3 x + a_4 \tag{3.66}$$

We need to compute four points (that bracket the minimum) for the estimation of the minimum, either four values of the polynomial $f(x)$, or the values of $f(x)$ and the derivative of $f(x)$, each at two points.

In the first case, we obtain four linear equations with the four unknown parameters (a_1, a_2, a_3, and a_4) that are the desired coefficients. Let the matrix X be represented as

$$X = \begin{bmatrix} x_1^3 & x_1^2 & x_1 & 1 \\ x_2^3 & x_2^2 & x_2 & 1 \\ x_3^3 & x_3^2 & x_3 & 1 \\ x_4^3 & x_4^2 & x_4 & 1 \end{bmatrix} \tag{3.67}$$

$$\mathrm{F}^T = \begin{bmatrix} f(x_1) & f(x_2) & f(x_3) & f(x_4) \end{bmatrix} \tag{3.68}$$

$$A^T = \begin{bmatrix} a_1 & a_2 & a_3 & a_4 \end{bmatrix} \tag{3.69}$$

$$F = XA \tag{3.70}$$

The extremum of $f(x)$ is obtained by setting the derivative of $f(x)$ equal to zero as shown in Eq. (3.71) and then solving for $\tilde{x}$

$$\frac{df(x)}{dx} = 3a_1x^2 + 2a_2x + a_3 = 0 \tag{3.71}$$

so that,

$$\tilde{x} = \frac{-2a_2 \pm \sqrt{4a_2^2 - 12a_1a_3}}{6a_1} \tag{3.72}$$

The sign of the second derivative of $f(\tilde{x})$ governs the sign to be used before the square root, that is to say, whether a minimum or maximum is sought. Equation (3.74) can be used to compute the vector A

$$F = XA \tag{3.73}$$

or $$A = X^{-1}F \tag{3.74}$$

After predicting the optimum point $\tilde{x}$, it is employed as a new point for the next iteration and the point with the highest value of $f(x)$ [lowest value of $f(x)$ for maximization] is eliminated.

When, the first derivatives of $f(x)$ are available, only two points are required, and the cubic function can be fitted to the two pairs of the slope values and function values. The four coefficients can be uniquely related to these four pieces of information in the cubic equation, which can be optimized to predict the new, nearly optimal data point. If $\left(x_1, f_1, f_1'\right)$ and $\left(x_2, f_2, f_2'\right)$ are available, then the optimum $\tilde{x}$ is

$$\tilde{x} = x_2 - \left[\frac{f_2' + w - z}{f_2' - f_1' + 2w}\right](x_2 - x_1) \tag{3.75}$$

where

$$z = \frac{3[f_1 - f_2]}{[x_2 - x_1]} + f_1' + f_2' \tag{3.76}$$

$$w = \left[z^2 - f_1'.f_2'\right]^{1/2} \tag{3.77}$$

In a minimization problem, we require $x_1 < x_2$, $f_1' < 0$, and $f_2' > 0$ (the minimum is bracketed by x_1 and x_2). Calculate the function value $f(\tilde{x})$ at the new point $(\tilde{x})$ to determine which of the previous two points to replace. The application of this technique for solving nonlinear programming problem that use gradient information is straightforward and efficient.

Summary

- This cheaper discusses various methods for optimization of single-variable. The criteria and conditions for this optimization are given in this chapter. This section provides some idea about different search methods like direct search and gradient search methods. Bracketing of the optimization point is very crucial for unimodal function; this technique is given in this chapter. Here, we have presented unrestricted search method, exhaustive search, dichotomous search, interval halving method, Fibonacci method, and golden section method. Beside this, Newton method, Quasi-Newton method, secant method and polynomial approximation methods are also considered.

Exercise

3.1 Why single-variable unconstrained optimization is important for chemical engineers? Give some examples of the single-variable unconstrained optimization problem.

3.2 What is the difference between interpolation and elimination methods?

3.3 Describe the Fibonacci numbers.

3.4 What is a unimodal function? What are the different methods for optimizing the unimodal function?

3.5 Use the quadratic interpolation method to find the minimum of the function given in Example 3.3. Consider the initial step size of 0.1.

3.6 Use the cubic interpolation method to find the minimum of the function given in Example 3.3. Consider an initial step size of $t_0 = 0.1$.

3.7 Prove that a convex function is unimodal.

3.8 Determine the value of x within the interval (0, 1) that minimizes the function $f = (x - 1)(x - 2.5)$ to within ± 0.025 by (a) the Fibonacci method and (b) the golden section method.

3.9 Find the minimum value of the function $f = x^4 - x + 1$ using secant method.

3.10 Write an algorithm for finding the minimum resistance of heat transfer using Eq. (2.50). Use Newton method for the same.

3.11 Solve the Example 3.3 using Quasi-Newton method.

References

Biggs, M. B. 2008. *Nonlinear Optimization with Engineering Applications*, Springer Optimization and its Applications, vol. 19.

Edgar, T. F., Himmelblau, D. M., Lasdon, L. S. *Optimization of Chemical Processes* (2*nd ed.*), McGraw–Hill.

Rao, S. S. *Engineering Optimization Theory and Practice* (4*e*), New Jersey: John Wiley and Sons, Inc.

Ravindran, A., Ragsdell, K. M., Reklaitis, G. V. *Engineering Optimization Methods and Applications* (2*e*), John Wiley and Sons, Inc.

Snyman, J. A. *Practical Mathematical Optimization*, Springer.